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Full Length Article

An Eulerian model for the simulation of the thermal conversion of a single large biomass particle

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ABSTRACT

This paper presents a comprehensive model for simulating the combustion of large biomass particles. The model implements a set of Eulerian variables that represent the components of solid biomass in a commercial CFD code. The evolution of these variables represents the thermal conversion of biomass and its interaction with the gas flow. The model consists of several reaction submodels of heat transfer and species diffusion. A wood shrinkage submodel was also proposed, and it acts locally in cells according to calculations of the consumption densities and globally in the particle according to mass and energy movements across the mesh. An experimental reactor, in which a biomass particle was irradiated with a xenon lamp, was modelled to simulate the drying and devolatilization stages under controlled conditions. Two documented experiments were simulated, and the predictions were compared with the experimental results. The temperature evolution of the particle at several depths was analysed, and a qualitative comparison of the particle shrinkage was performed. The comparison yielded reasonably good predictions for temperatures inside the particle and similar trends in log shrinkage despite some uncertainties regarding the biomass composition and experimental conditions.

1. Introduction

The lack of fossil fuel resources in numerous European countries and the growing need for investments in renewable energies have made biomass combustion an important field of research in recent decades. Advances in computational techniques have contributed to the study of different processes in combustion science via modelling and simulation tools that aid in predicting and understanding combustion phenomena. However, these techniques require significant development for application to solid biomass combustion since they cannot simulate the complex conversion, transport and reaction processes in the biphasic medium in a boiler or burner.

The main difficulty is the thermal conversion of solid biomass since CFD techniques are highly efficient at modelling gas combustion. Researchers have proposed a wide variety of strategies to implement submodels for the conversion of solid biomass in CFD codes. Most of these works have focused on beds of small particles or grates of straw. The simplest approach is the zero-dimensional bed [1–5], which uses mass, energy and species balances to predict the species and energy emitted by the bed during the conversion. Another typical strategy is the walking column, a one-dimensional approach commonly used for the simulation of grates of straw [6–9] that models the transient advance of biomass in a grate through the steady exchange of mass and energy between the bed columns. Some models have achieved a higher level of geometrical discretization and a better resolution for combustion stages using two-dimensional [10] and three-dimensional beds [11–15]. These models have obtained the best results when the internal gradients of particles have been considered, i.e., a thermally thick approach and a separation of the combustion stages inside the particles [16–19]. Integration of discrete element model (DEM) with CFD has contributed to highly detailed models for the simulation of packed beds. Mahmoudi et al. [20] applied this approach to a grate obtaining a good agreement with experimental measurements. Wiese et al. [21] also applied a DEM model in a pellet stove and simulated complex particle shapes for thermally thick biomass particles in a multi particles approach.

Most studies have been performed in packed or fluidized beds of small particles. However, modelling large wood particles is still a challenge due to the need to increase the number of grid points inside the particles. Porteiro et al. [22] used a one-dimensional internal discretization in 25 layers combined with a shrinkage scheme based on an elementary cell analogy that considers the particle shrinkage and growing internal porosity. Babu and Chaurasia [23] calculated the heat transfer inside the particle subgrid with a tri-diagonal matrix algorithm

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Nomenclature

A_i	Pre-exponential factor (s^{-1})
A_{fi}	Area of face i (m^2)
A_v	Area-volume ratio (m^{-1})
C_p	Specific heat ($J{\cdot}kg^{-1}{\cdot}K^{-1}$)
C_μ	k-ε model constant
d	Diameter (m)
Di_i	Diffusivity of the species i in the mixture ($m^2{\cdot}s^{-1}$)
E	Surface constant for the law of the wall (−)
E_i	Activation energy ($J{\cdot}mol^{-1}$)
h	Convection coefficient ($W{\cdot}m^{-2}{\cdot}K^{-1}$)
h_s	Solid phase enthalpy ($J{\cdot}kg^{-1}$)
k	Thermal conductivity ($W{\cdot}m^{-1}{\cdot}K^{-1}$)
k_{turb}	Turbulent kinetic energy ($m^2{\cdot}s^{-2}$)
$k_\perp$	Thermal conductivity perpendicular to fibres
K	Char reaction constants ($m{\cdot}s^{-1}$)
k_m	Mass transfer constant ($m{\cdot}s^{-1}$)
LH	Latent heat ($J{\cdot}kg^{-1}$)
M_i	Molecular weight ($kg{\cdot}kmol^{-1}$)
$\vec{r}$	Position vector (m)
R	Ideal gas constant ($J{\cdot}K^{-1}{\cdot}mol^{-1}$)
Nu	Nuselt number (−)
Pr	Prandtl number (−)
Sh	Sherwood number (−)
Sc	Schmidt number (−)
S	Source term ($W{\cdot}m^{-3}$)
T	Temperature (K)
T^+	Dimensionless temperature for the function of the wall (−)
t	Time (s)
V	Volume (m^3)
u^+	Law of the wall, dimensionless velocity (−)
v_∞	Gas velocity ($m{\cdot}s^{-1}$)
$\vec{v}_{shr}$	Shrinkage direction vector (m)
X	Volumetric fraction (−)
Y	Mass fraction (−)
y_{node}	Distance from the wall to the node (m)
y^+	Dimensionless distance to the wall (−)

Greek

Γ	Tortuosity (−)
$\Gamma_{\perp/\parallel}$	Ratio of perpendicular to parallel thermal conductivity (−)
ε	Solid fraction (−)
ε m	Emissivity (−)
η	Permeability (m^2)
κ	von Karman constant (−)
μ	Dynamic viscosity ($kg{\cdot}m^{-1}\,s^{-1}$)
ν	Kinematic viscosity ($m^2{\cdot}s^{-1}$)
ρ	Density ($kg{\cdot}m^{-3}$)
τ	Fraction of heat received by the particle employed in drying (−)
τ_w	Wall shear stress ($kg{\cdot}m^{-2}{\cdot}s^{-1}$)
$\Upsilon_{\perp/\parallel}$	Ratio of perpendicular to parallel permeability (−)
φ	Char oxidation parameter (−)
$\dot{\omega}_i'''$	Generation or consumption rate of the wood components ($kg{\cdot}m^{-3}{\cdot}s^{-1}$)

Subscripts

C	Carbon
c	Consumption
col	Collapse
eff	Effective
DC	Discharging cell
g	Gas
G	Generation
glob	Global
int	Internal
lam	Laminar
moist	Moisture
RC	Receiving cell
part	Particle
s	Solid
turb	Turbulent
wood	Dry wood

Superscripts

g,1	Gasification reaction with CO_2
g,2	Gasification reaction with H_2O
ox	Char oxidation
s	Specific

that is based on classical techniques used in numerical heat transfer theory [24]. Lu et al. [25] also discretized biomass particles in several layers and simulated several combustion phenomena, such as drying, rapid pyrolysis, gasification, and char oxidation processes, using a model that is applicable to different geometrical shapes and that considers the surroundings of a particle. This work demonstrates that the commonly used spherical approximations for nonspherical particles are not applicable to large sizes. To reduce the high computational cost, Thunman et al. [26] proposed an Eulerian approach that reduces the number of grid points to a few layers that represent the stages in biomass thermal conversion. This approach has been applied by several authors [16–19] for packed beds; however, all of the studies have focused on relatively small particles. Grønli and Melaaen [27] also used finite volume discretization to model logs of different biomass species and tested the model using an experimental reactor. The authors discretized cylindrical trunks along the main length using a simplified one-dimensional model and produced reasonably good results. Shi et al. [28] used a three-dimensional model to calculate the pyrolysis reactions of biomass particles via finite element techniques. They applied the model to one-centimetre-sized particles; however, the model is applicable to larger particles. Okekunle et al. [29] also modelled heat transfer and wood pyrolysis reactions inside particles using a finite volume approach. Soria et al. [30] proposed a two-dimensional model for single particles that calculates the thermal conversion of particles considering the heat, mass and species transport inside the particle porous structure. The model results were in good agreement with experiments performed using a solar radiation concentrator.

In this study, a numerical model is implemented in CFD code to simulate large biomass particles. A three-dimensional discretization is applied in the region of solid biomass, and a set of Eulerian variables are defined to model the main parameters of the solid phase. The evolution of these variables defines the state of biomass degradation and the stage of combustion. The gas phase is also calculated in the particle region using a porous formulation. A complete reaction scheme is used to model both the biomass thermal conversion and gas reactions. Heat transfer through the solid phase, the interaction with the gas phase and the diffusion of mass and species through the biomass porous structure are detail. The model also includes a particle shrinkage submodel that accounts for the contraction suffered by the entire biomass piece during conversion through mass and energy movements across